

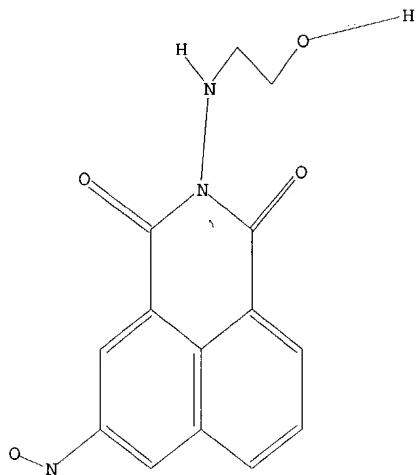
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L2 STRUCTURE UPLOADED

=> d

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l2

SAMPLE SEARCH INITIATED 11:36:09 FILE 'BEILSTEIN'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

=> s l2 sss full

FULL SEARCH INITIATED 11:36:19 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS
SEARCH TIME: 00.00.03

0 ANSWERS

L4 0 SEA SSS FUL L2

=>

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=> s e3

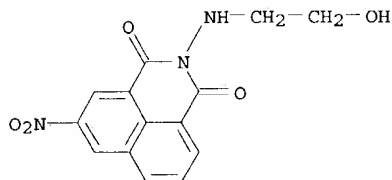
L1 1 234779-34-1/RN

=> d all

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 234779-34-1 REGISTRY
 ED Entered STN: 25 Aug 1999
 CN 1H-Benz[de]isoquinoline-1,3(2H)-dione, 2-[(2-hydroxyethyl)amino]-5-nitro-
 (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN ALE 0540
 FS 3D CONCORD
 MF C14 H11 N3 O5
 SR CA
 LC STN Files: BIOSIS, CA, CAPLUS, CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N-C6-C6	NC5-C6-C6	6-6-6	C12N	1784.14.8	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1	pH 10	(1) ACD
Boiling Point (BP)	553.0+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	87.73+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	288.3+/-59.2 deg C		(1) ACD
H acceptors (HAC)	8		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	34.2	pH 1	(1) ACD
Koc (KOC)	34.2	pH 4	(1) ACD
Koc (KOC)	34.2	pH 7	(1) ACD
Koc (KOC)	34.2	pH 8	(1) ACD
Koc (KOC)	34.2	pH 10	(1) ACD
logD (LOGD)	0.29	pH 1	(1) ACD
logD (LOGD)	0.29	pH 4	(1) ACD
logD (LOGD)	0.29	pH 7	(1) ACD
logD (LOGD)	0.29	pH 8	(1) ACD
logD (LOGD)	0.29	pH 10	(1) ACD
logP (LOGP)	0.290+/-0.626		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	301.25		(1) ACD
Vapor Pressure (VP)	4.59E-13 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
 Solaris V4.67 ((C) 1994-2004 ACD/Labs)

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See HELP PROPERTIES for information about property data sources in REGISTRY.
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 135:298810 CA
TI Use of NGF antagonists for the prevention or treatment of chronic visceral pain
IN Diop, Laurent; Delafoy, Laure
PA Warner-Lambert Company, USA
SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-00
ICS A61K031-473; A61K039-395; A61P015-00; A61P001-06; A61P001-18; A61P001-14; A61P001-00
CC 1-11 (Pharmacology)
Section cross-reference(s): 2, 63

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001078698	A2	20011025	WO 2001-EP3490	20010326
	W:		AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
	RW:		GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
	FR 2807660	A1	20011019	FR 2000-4782	20000413
	EP 1282421	A2	20030212	EP 2001-927818	20010326
	R:		AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR		
	BR 2001010028	A	20030603	BR 2001-10028	20010326
	JP 2003530427	T2	20031014	JP 2001-575999	20010326
PRAI	FR 2000-4782		20000413		
	WO 2001-EP3490		20010326		
AB	A nerve growth factor (NGF) antagonist is used for the manufacture of a medicament intended for the prevention or treatment of chronic visceral pain. Corresponding pharmaceutical comps. are also disclosed.				
ST	NGF antagonist chronic visceral pain treatment				
IT	Analgesics				
	Drug delivery systems				
	Dysmenorrhea				
	Dyspepsia				
	(NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Nerve growth factor receptors				
	RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)				
	(NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Pain				
	(chronic; NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Digestive tract				
	(gastroesophageal reflux; NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Intestine, disease				
	(irritable bowel syndrome; NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Drug delivery systems				
	(oral; NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Viscera				
	(pain; NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Pancreas, disease				
	(pancreatitis; NGF antagonists for prevention or treatment of chronic visceral pain)				
IT	Antibodies				
	RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)				
	(to NGF; NGF antagonists for prevention or treatment of chronic				

visceral pain)
 IT Viscera
 (visceralgia; NGF antagonists for prevention or treatment of chronic visceral pain)
 IT 234779-34-1, ALE 0540
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (NGF antagonists for prevention or treatment of chronic visceral pain)
 IT 137010-36-7, NGF receptor tyrosine kinase
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
 (NGF antagonists for prevention or treatment of chronic visceral pain)
 IT 9061-61-4, Nerve growth factor
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (NGF antagonists for prevention or treatment of chronic visceral pain)

REFERENCE 2

AN 131:125331 CA
 TI Characterization of antiallodynic actions of ALE-0540, a novel nerve growth factor receptor antagonist, in the rat
 AU Owolabi, Joshua B.; Rizkalla, Geihan; Tehim, Ashok; Ross, Gregory M.; Riopelle, Richard J.; Kamboj, Rajender; Ossipov, Michael; Bian, Di; Wegert, Sandara; Porreca, Frank; Lee, David K. H.
 CS Allelix Biopharmaceuticals Inc., Mississauga, Can.
 SO Journal of Pharmacology and Experimental Therapeutics (1999), 289(3), 1271-1276
 CODEN: JPETAB; ISSN: 0022-3565
 PB American Society for Pharmacology and Experimental Therapeutics
 DT Journal
 LA English
 CC 1-11 (Pharmacology)
 AB There is growing evidence that nerve growth factor (NGF) may function as a mediator of persistent pain states. We have identified a novel nonpeptidic mol., ALE-0540, that inhibits the binding of NGF to tyrosine kinase (Trk) A or both p75 and TrkA (IC₅₀ 5.88±1.87 µM, 3.72±1.3 µM, resp.), as well as signal transduction and biol. responses mediated by TrkA receptors. ALE-0540 was tested in models of neuropathic pain and thermally-induced inflammatory pain, using two routes of administration, a systemic i.p. and a spinal intrathecal (i.t.) route. Morphine was also tested for comparison in the antiallodynia model using mech. stimuli. We show that either i.p. or i.t. administration of ALE-0540 in rats produced antiallodynia in the L5/L6 ligation model of neuropathic pain. The calculated A50 values (and 95% confidence intervals) for ALE-0540 administered i.p. and i.t. were 38 (17.5-83) mg/kg and 34.6 (17.3-69.4) µg, resp. ALE-0540 given i.t., at doses of 30 and 60 µg, also blocked tactile allodynia in the thermal sensitization model. Although morphine displayed greater potency [A50 value of 7.1 (5.6-8.8) mg/kg] than ALE-0540 in anti-allodynic effect when given i.p. to L5/L6-ligated rats, it was not active when administered i.t. These data suggest that a blockade of NGF bioactivity using a NGF receptor antagonist is capable of blocking neuropathic and inflammatory pain and further support the hypothesis that NGF is involved in signaling pathways associated with these pain states. ALE-0540 represents a nonpeptidic small mol. which can be used to examine mechanisms leading to the development of agents for the treatment of pain.
 ST ALE 0540 antiallodynia nerve growth factor
 IT Pain
 Skin, disease
 (allodynia; characterization of antiallodynic actions of ALE-0540, a novel nerve growth factor receptor antagonist, in the rat)
 IT Analgesics
 (characterization of antiallodynic actions of ALE-0540, a novel nerve growth factor receptor antagonist, in the rat)
 IT Nerve growth factor receptors
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (characterization of antiallodynic actions of ALE-0540, a novel nerve growth factor receptor antagonist, in the rat)
 IT 234779-34-1, ALE 0540
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (characterization of antiallodynic actions of ALE-0540, a novel nerve growth factor receptor antagonist, in the rat)
 IT 9061-61-4, Nerve growth factor
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (characterization of antiallodynic actions of ALE-0540, a novel nerve growth factor receptor antagonist, in the rat)

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RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD

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